Weak pseudogap behavior in the underdoped cuprate superconductors

Jörg Schmalian,[a] David Pines,[a,b] and Branko Stojković[b]
[a] University of Illinois at Urbana-Champaign, Loomis Laboratory of Physics, 1110 W. Green, Urbana, IL, 61801
[b] Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM, 87545
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We report on an exact solution of the nearly antiferromagnetic Fermi liquid spin fermion model in the limit $\pi T \gg \omega_{\rm sf}$, which demonstrates that the broad high energy features found in ARPES measurements of the spectral density of the underdoped cuprate superconductors are determined by strong antiferromagnetic (AF) correlations and precursor effects of an SDW state. We show that the onset temperature, $T^{\rm cr}$, of weak pseudo-gap (pseudoscaling) behavior is determined by the strength, ξ, of the AF correlations, and obtain the generic changes in low frequency magnetic behavior seen in NMR experiments with $\xi(T^{\rm cr}) \approx 2$, confirming the Barzykin and Pines crossover criterion.

74.25.-q,75.25.Dw,74.25.Ha

Magnetically underdoped cuprates may be distinguished from their overdoped counterparts by the presence of a maximum at a temperature $T^{\rm cr} > T_c$ in the temperature dependent uniform susceptibility, $\chi_o(T)$. They are characterized by the occurrence of a quasiparticle pseudogap observed by NMR and INS experiments, optical, transport and specific heat measurements, and in angular resolved photoemission spectroscopy (ARPES). Barzykin and Pines [1] proposed that at $T^{\rm cr}$, sizable AF correlations between the planar quasiparticles bring about a change in the spin dynamics, and that at T near $T^{\rm cr}$, the quantity ${}^{63}T_1T/{}^{63}T_{2\rm G}^2$, where ${}^{63}T_1$ is the ^{63}Cu spin-lattice relaxation time and ${}^{63}T_{2\rm G}$ is the spin-echo decay time, changes from being nearly independent of temperature (above $T^{\rm cr}$), to a quantity which varies as $(a+bT)^{-1}$. This behavior has recently been confirmed in NMR measurements by Curro *et al.* [2]. Since ${}^{63}T_1T/{}^{63}T_{2\rm G}^n \propto \xi^{n-z}$, where z is a dynamical exponent [1], the near temperature independence of ${}^{63}T_1T/{}^{63}T_{2\rm G}$ found between $T^{\rm cr}$ and a lower crossover temperature, T_*, suggests that one is in a pseudoscaling regime ($z \approx 1$), while the temperature independence of of ${}^{63}T_1T/{}^{63}T_{2\rm G}^2$ above $T^{\rm cr}$ suggests mean field behavior ($z \approx 2$). Moreover, above T_* ARPES experiments show that the spectral density of quasiparticles located near $(\pi,0)$ has developed a high energy feature [3]. We refer to this behavior as *weak pseudogap behavior*, to distinguish it from the *strong pseudogap behavior* found below T_*, where experiment shows a leading edge gap develops in the quasiparticle spectrum [3]. Strong pseudogap behavior is also seen in specific heat, d.c. transport, and optical experiments, while ${}^{63}T_{2\rm G}$ measurements show that the AF spin correlations become frozen (i.e., $\xi \approx$ *const.*) and ${}^{63}T_1T$ displays gap-like behavior.

The nearly antiferromagnetic Fermi liquid (NAFL) model [4,5] of the cuprates offers a possible explanation for the observed weak and strong pseudogap behavior. In this model, changes in quasiparticle behavior both reflect and bring about the measured changes in spin dynamics. The highly anisotropic effective planar quasiparticle interaction mirrors the dynamical spin susceptibility, peaked near $\mathbf{Q} = (\pi.\pi)$, introduced by Millis, Monien, and Pines [6] to explain NMR experiments:

$$V_{\rm eff}^{\rm NAFL}(\mathbf{q},\omega) = g^2\chi_{\mathbf{q}}(\omega) = \frac{g^2\chi_{\mathbf{Q}}}{1+\xi^2(\mathbf{q}-\mathbf{Q})^2 - i\frac{\omega}{\omega_{\rm sf}}}\,, \quad (1)$$

where $\chi_{\mathbf{Q}} = \alpha\xi^2$, with α constant, and g is the coupling constant.

Since the dynamical spin susceptibility $\chi_{\mathbf{q}}(\omega)$ peaks at wave vectors close to (π,π), two different kinds of quasiparticles emerge: *hot quasiparticles*, located close to those momentum points on the Fermi surface which can be connected by $\mathbf{Q}$, feel the full effects of the interaction of Eq.1; *cold quasiparticles*, located not far from the diagonals, $|k_x| = |k_y|$, feel a "normal" interaction. Their distinct lifetimes can be inferred from transport experiments, where a detailed analysis shows that the behavior of the hot quasiparticles is highly anomalous, while cold quasiparticles may be characterized as a strongly coupled Landau Fermi Liquid [7].

In the present communication we focus our attention on temperatures $T \geq T_*$. Our reason for doing so is that for $T > T_*$, fits to NMR experiments show that $\omega_{\rm sf} < \pi T$, the frequency equivalent of temperature. Because of its comparatively low characteristic energy the spin system is thermally excited and behaves quasistatically; the hot quasiparticles see a spin system which acts like a static deformation potential, a behavior which is no longer found below T_* where the lowest scale is the temperature itself and the quantum nature of the spin degrees of freedom is essential. We find that above T_*, in the limit $\pi T \gg \omega_{\rm sf}$ it is possible to obtain an exact solution of the spin fermion model with the effective interaction, $V_{\rm eff.}^{\rm NAFL}(\mathbf{q},\omega)$, of Eq. 1.

Our main results are the appearance in the hot quasiparticle spectrum of the high energy features seen in ARPES, a maximum in $\chi_o(T)$ and a crossover in ${}^{63}T_1T/{}^{63}T_{2\rm G}^2$ for $\xi > \xi_o \approx v_{\rm F}/\Delta_o$. These are produced

by the emergence of an SDW-like state, as proposed by Chubukov *et al.* [8] Here, $v_{\rm F}$ is the Fermi velocity and $\Delta_o = \frac{g}{\sqrt{3}}\sqrt{\langle \mathbf{S}^2\rangle} \sim \frac{g}{2}$, a characteristic energy scale of the SDW-like pseudogap. Using typical values for the hopping elements (see below), and $g \approx 0.6\,\mathrm{eV}$ (determined from the analysis of transport experiments in slightly underdoped materials [7]), we find $\xi_0 \approx 2$. For $\xi > \xi_o$, the hot quasiparticle spectral density takes a two-peak form which reflects the emerging spin density wave state, while the MMP interaction generates naturally the distinct behavior of hot and cold quasiparticle states seen in ARPES experiments.

Before discussing these results, we summarize our calculations briefly. Using the effective interaction, Eq. 1, the direct spin-spin coupling is eliminated via a Hubbard-Stratonovich transformation, introducing a collective spin field $\mathbf{S}_{\mathbf{q}}(\tau)$. After integrating out the fermionic degrees of freedom, the single particle Green's function can be written as

$$G_{\mathbf{k},\sigma}(\tau-\tau') = \left\langle \hat{G}_{\mathbf{k},\mathbf{k}\sigma\sigma}(\tau,\tau'|\mathbf{S})\right\rangle_o , \qquad (2)$$

where $\hat{G}_{\mathbf{k},\mathbf{k}\sigma\sigma}(\tau,\tau'|\mathbf{S})$ is the matrix element of

$$[G^{-1}_{o\mathbf{k}}(\tau-\tau')\delta_{\mathbf{k},\mathbf{k}'} - \frac{g}{\sqrt{3}}\mathbf{S}_{\mathbf{k}-\mathbf{k}'}(\tau)\delta(\tau-\tau')\cdot\vec{\sigma}]^{-1}, \qquad (3)$$

which describes the propagation of an electron for a given configuration $\mathbf{S}$ of the spin field. $\vec{\sigma}$ is the Pauli matrix vector and $G^{-1}_{o\mathbf{k}} = -(\partial_\tau + \varepsilon_{\mathbf{k}})$ is the inverse of the unperturbed single particle Green's function with bare dispersion

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t'\cos k_x \cos k_y - \mu\,. \qquad (4)$$

In the following we use $t = 0.25\,\mathrm{eV}$ and $t' = -0.4t$ for the nearest and next nearest neighbor hopping integrals, respectively, and we adjust the chemical potential μ to maintain the constant hole concentration at $n_h = 15\%$. The average $\langle\cdots\rangle_o = \frac{1}{Z_{\rm B}}\int \mathcal{D}\mathbf{S}\cdots\exp\{-S_o\}$ is performed with respect to the action of the collective spin degrees of freedom:

$$S_o(\mathbf{S}) = \frac{T}{2}\sum_{\mathbf{q},n}\chi^{-1}_{\mathbf{q}}(i\omega_n)\,\mathbf{S}_{\mathbf{q}}(i\omega_n)\cdot\mathbf{S}_{-\mathbf{q}}(-i\omega_n) \qquad (5)$$

where $\omega_n = 2n\pi T$ and $Z_{\rm B}$ is defined via $\langle 1\rangle_o = 1$. In using Eq. 2 we have assumed that (*i*) $\chi_{\mathbf{q}}(\omega)$ is the fully renormalized spin-susceptibility taken from the experiment and (*ii*) any nonlinear (higher order in $\mathbf{S}$ than quadratic) terms of the spin field can be neglected. The model which results from assumption (*ii*) is usually referred to as the spin fermion model.

After inversion of Eq. 3 in spin space, the average of Eq. 2 can be evaluated diagrammatically using Wick's theorem for the spin field. In the above mentioned static limit, $\pi T \gg \omega_{\rm sf}$, it suffices to consider only the zeroth bosonic Matsubara frequency in $\chi_{\mathbf{q}}(i\omega_n)$. The remaining momentum summations are evaluated by expanding $\varepsilon_{\mathbf{k}+\mathbf{q}} \approx \varepsilon_{\mathbf{k}+\mathbf{Q}} + \mathbf{v}_{\mathbf{k}+\mathbf{Q}}\cdot(\mathbf{q}-\mathbf{Q})$ for momentum transfers close to $\mathbf{Q}$, using $v^{\alpha}_{\mathbf{k}+\mathbf{Q}} = \partial\varepsilon_{\mathbf{k}+\mathbf{Q}}/\partial k_\alpha$. In this limit *all diagrams* can be summed up by generalizing a solution for a one dimensional charge density wave system obtained by Sadovskii [9] to the case of two dimensions, and more importantly, to isotropic spin fluctuations. We find the following recursion relation for the Green's function $G_{\mathbf{k}}(\omega) \equiv G^{l=0}_{\mathbf{k}}(\omega)$, whose imaginary part determines the spectral density $A(\mathbf{k},\omega)$, seen in ARPES [10]:

$$[G^l_{\mathbf{k}}(\omega)]^{-1} = \omega - \varepsilon_{\mathbf{k}+l\mathbf{Q}} + i\frac{l v_{\mathbf{k},l}}{\xi} - \kappa_{l+1}\Delta_o^2 G^{l+1}_{\mathbf{k}}(\omega). \qquad (6)$$

Here, $v_{\mathbf{k},l} = |\mathbf{v}_{\mathbf{k}+\mathbf{Q}}|$ and $\kappa_l = (l+2)/3$ if l is odd, while $v_{\mathbf{k},l} = |\mathbf{v}_{\mathbf{k}+\mathbf{Q}}|(|\cos\phi_{\mathbf{k}}| + |\sin\phi_{\mathbf{k}}|)$ and $\kappa_l = l/3$ if l is even. $\phi_{\mathbf{k}}$ is the angle between $\mathbf{v}_{\mathbf{k}+\mathbf{Q}}$ and $\mathbf{v}_{\mathbf{k}}$. The recursion relation, Eq. (6), enables us to calculate $A(\mathbf{k},\omega)$ to arbitrary order in the coupling constant g. In the limit $\xi \to \infty$ the Green's function reduces to $G_{\mathbf{k}}(\omega) = \int d\Delta\ p(\Delta)\ G^{\rm SDW}_{\mathbf{k}}(\Delta)$, where $G^{\rm SDW}_{\mathbf{k}}(\Delta)$ is the single particle Green's function of the mean field SDW state and $p(\Delta) \sim \Delta^2\exp(-\frac{3}{2}\Delta^2/\Delta_0^2)$ is the distribution function of a fluctuating SDW gap, centered around $\sqrt{\frac{2}{3}}\Delta_0$, i.e., the amplitude fluctuations of the spins $\mathbf{S}$ are confined to a region around $\sqrt{\frac{2}{3}\langle\mathbf{S}^2\rangle}$, although in our calculations directional fluctuations are fully isotropic and spin rotation invariance is maintained. Below we show that the SDW like solution is obtained even at finite values of ξ.

The quantities we calculate are the single particle spectral density, $A(\mathbf{k},\omega)$ and the low frequency behavior of the irreducible spin susceptibility $\tilde{\chi}_{\mathbf{q}}(\omega,T)$. Our principal results are depicted in Figures 1-3. The ξ-dependence of the Fermi surface, shown in the inset to Fig. 1a, is similar to the results obtained by Chubukov *et al.* [11] at $T = 0$; however for the experimentally relevant range of ξ, hole pockets around $\mathbf{k} = (\pi/2,\pi/2)$ do not form. We have used the criterion $\varepsilon_{\mathbf{k}} + \mathrm{Re}\Sigma_{\mathbf{k}}(\omega=0) = 0$ to determine the Fermi surface. Although strictly valid only for $T = 0$, for finite temperatures it indicates when a quasiparticle crosses the chemical potential. In the limit of very large correlation length, we find, in addition to the two broadened poles of a SDW like state, a third solution of $\omega = \mathrm{Re}\Sigma_{\mathbf{k}}(\omega) + \varepsilon_{\mathbf{k}}$, which although not visible due to the large scattering rates, ensures that even for $\xi \to \infty$ a large Fermi surface and only a pseudogap in the density of states occur.

A comparatively sharp transition between the behavior of hot quasiparticles (located at points a and b on the Fermi surface of Fig. 1a) and cold quasiparticles (at d and e) is found. For hot quasiparticles the single particle spectral density evolves with temperature as the AF correlation length increases from $\xi \approx 1$ to 5; a two

peak structure, which corresponds to a transfer of spectral weight from low frequencies to frequencies above $200 - 300\,\mathrm{meV}$, develops at $\xi_o \approx 2$, and is quite pronounced for $\xi \geq 3$ (Fig. 1b). As may be seen in Fig. 1a, the shift in spectral density found for hot quasiparticles does not occur for cold quasiparticles, whose spectral density continues to be peaked at the Fermi energy.

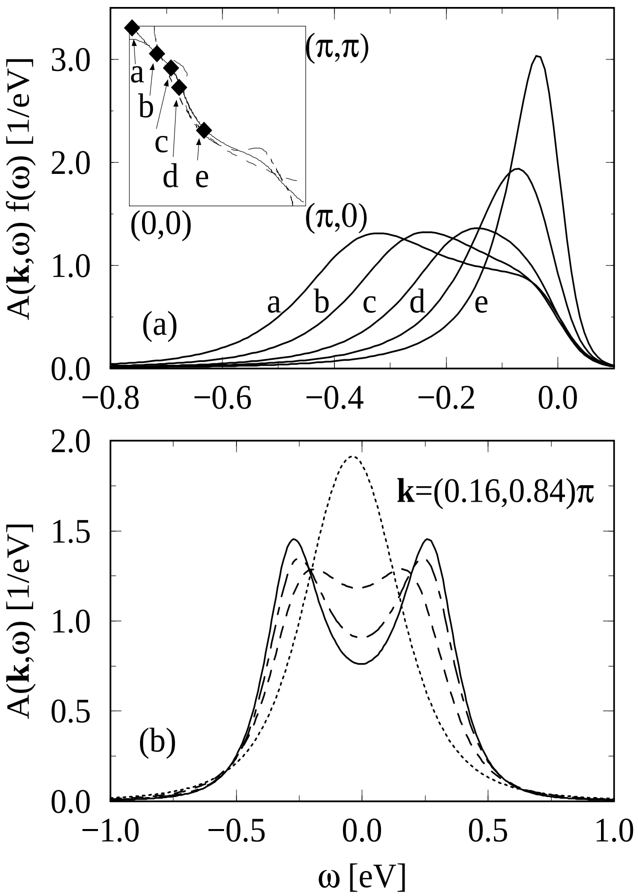

FIG. 1. (a) Spectral density multiplied with Fermi function on the Fermi surface for $\xi = 3$. The distinct behavior of hot and cold quasiparticles is visible. The inset shows the corresponding Fermi surface and its ξ-dependence. The dashed, solid and dashed-dotted lines correspond to $\xi = 1$, 3 and 10, respectively. (b) ξ-dependence of the spectral density of point b in (a). The transition from a conventional line shape for small $\xi = 1$ (dotted line) to spectral densities with broad lines and pronounced high energy features ($\xi = 2, 3$, and 5 for the dashed, dashed dotted, and solid line, respectively), reflecting a precursor SDW state, is visible. Note, the saturation of the precursor effects for $\xi \approx 3$.

We sum *all diagrams* of the perturbation series for the electron-spin fluctuation vertex function in similar fashion as the Green's function $G_{\mathbf{k}}(\omega)$ in Eq. (6). The lack of symmetry breaking is essential for a proper evaluation of the vertex which, as long as the spin rotation invariance is intact, is reduced at most by a factor $\approx \frac{1}{3}$ for the high energy features [11,12]. For lower excitation energies, this vertex is considerably enhanced for the hot quasiparticles; it is almost unaffected for the cold quasiparticles, reflecting again their qualitatively different behavior.

We combine the results for $G_{\mathbf{k}}(\omega)$ and the electron-spin fluctuation vertex function and so determine the irreducible spin susceptibility $\tilde{\chi}_{\mathbf{q}}(\omega)$. We find (Fig. 2) that both $\tilde{\chi}_o(T)$ and $\tilde{\chi}_{\mathbf{Q}}(T)$ exhibit maxima at temperatures close to $T^{\rm cr}$ where $\xi \approx 2$. In these calculations we assumed that $\xi^{-1}(T) = \frac{1}{4} + \frac{1}{4}\frac{T-T_*}{T^{\rm cr}-T_*}$ between $T^{\rm cr} = 470\,\mathrm{K}$ and $T_* = 220\,\mathrm{K}$ and $\xi^{-2}(T) = \frac{1}{4} + \frac{1}{7}\frac{T-T^{\rm cr}}{700\,\mathrm{K}-T^{\rm cr}}$ above $T^{\rm cr}$ consistent with the NMR results of Curro *et al.* [2] for $\mathrm{YBa_2Cu_4O_8}$. The behavior of $\tilde{\chi}_o(T)$ and $\tilde{\chi}_{\mathbf{Q}}(T)$ above the maximum reflects the increasing importance of lifetime (strong coupling) effects which act to reduce both irreducible susceptibilities. Because of comparatively short correlation lengths ($\xi < 2$), it is likely that Eliashberg calculations [5] will provide a better quantitative account in this mean field regime. The fall-off in $\tilde{\chi}_o(T)$ and $\tilde{\chi}_{\mathbf{Q}}(T)$ below $T^{\rm cr}$ arises primarily from the transfer of quasiparticle spectral weight to higher energies.

The determination of the full spin susceptibility $\chi_{\mathbf{q}}(\omega) = \tilde{\chi}_{\mathbf{q}}(\omega)/(1 - J_{\mathbf{q}}\tilde{\chi}_{\mathbf{q}}(\omega))$ requires calculating the restoring force $J_{\mathbf{q}}$, and is beyond the scope of the present work, since $J_{\mathbf{q}}$ is determined by the renormalization of the spin exchange fermion-fermion interaction through high energy excitations in all other channels. However, for $\chi_o(T)$, with the assumption that $J_{\mathbf{q}=0}\tilde{\chi}_0(T_{cr}) = 0.5$, a good quantitative fit to the experimental results of Curro *et al.* [2] between $T^{\rm cr}$ and T_* is found.

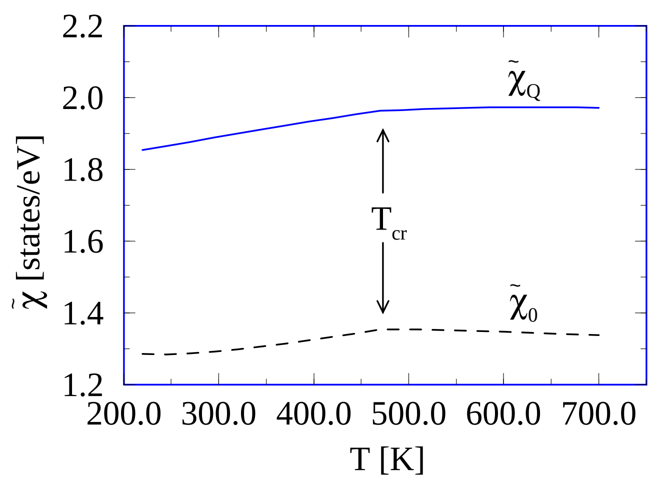

FIG. 2. Irreducible part $\tilde{\chi}_{\mathbf{q}}(T)$ of the static spin susceptibility at $\mathbf{q} = (0,0)$ and $\mathbf{q} = (\pi,\pi)$ as function of temperature.

We find that both vertex corrections and quasiparticle spectral weight transfer play a significant role in determining the low frequency spin dynamics. As may be seen in the inset to Fig. 3, when both effects are taken into account, our calculated values of the spin damping $\gamma_{\mathbf{Q}} = \tilde{\chi}''_{\mathbf{Q}}(\omega,T)/\omega\big|_{\omega=0}$ display the crossover at $T^{\rm cr}$ anticipated by Monthoux and Pines [13]. A second calcu-

lable quantity which can be compared with experiment is $\tilde{\chi}_{\mathbf{Q}}(T)^2/\gamma_{\mathbf{Q}} \equiv \omega_{sf}\chi_{\mathbf{Q}}$, being proportional to the product, ${}^{63}T_1T/({}^{63}T_{2\mathrm{G}})^2$. As may seen in Fig. 3, qualitative agreement with the results of Curro *et al.* [2] for $\mathrm{YBa_2Cu_4O_8}$ is found.

Physically, the most interesting aspect of our results is the appearance of SDW precursor phenomena, brought about by the strong interaction between the planar quasiparticles, for moderate AF correlation lengths, $\xi > \xi_o \approx 2$, in contrast to earlier calculations, in which SDW precursor behavior was only found in the limit of very large correlation length [14]. Our exact solution of the static problem enables us to access this region of strong coupling. For $\xi > \xi_o$, the hot electron mean free path, $\sim \xi_o^2/\xi$ begins to be small compared to ξ, so that the quasi particle can no longer distinguish the actual situation from that of a SDW state; hence we find pseudo-SDW behavior, i.e. SDW behavior without symmetry breaking. The related shift of spectral weight for states close to $(\pi, 0)$ affects mostly the low frequency part of the irreducible spin susceptibility and leads to the calculated crossover behavior. Because symmetry is not broken, there will continue to be coherent states at the Fermi energy; although their spectral weight is small one still has a large Fermi surface. Such coherent quasiparticles, invisible in the present temperature range, are, we believe, responsible for the sharp peak for $\mathbf{k} \sim (\pi, 0)$, observed in ARPES below the superconducting transition temperature [3].

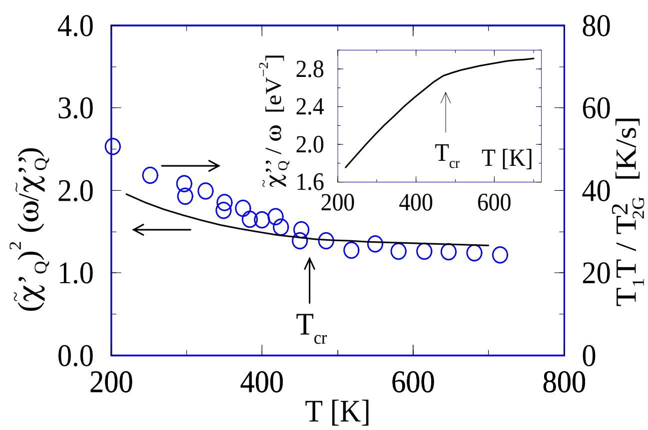

FIG. 3. $\tilde{\chi}_{\mathbf{Q}}^2\omega/\tilde{\chi}''_{\mathbf{Q}}\big|_{\omega=0}$ as function of temperature, compared with experimental results of Ref.[2] for $T_1T/T_{2\mathrm{G}}^2$. The inset shows the crossover in the calculated T-dependence of $\tilde{\chi}''_{\mathbf{Q}}(\omega)/\omega\big|_{\omega=0}$.

The present theory cannot, of course, explain the leading edge pseudogap found below T_*, since one is then no longer in the quasistatic limit for which our calculations apply. Strong pseudogap behavior corresponds to a further redistribution of quasiparticle states lying within $\approx 30\,\mathrm{meV}$ of the Fermi energy. No appreciable change is seen in the high energy features found in the present calculations. It is likely that strong scattering in the particle-particle channel plays an increasingly important role below T_*, since we find above T_* important prerequisites for its appearance; an enhanced spin fluctuation vertex and a pronounced flattening of the low energy part of the hot quasiparticle states [15]. In addition, below T_* the quantum behavior of spin excitations becomes increasingly important. This reduces the phase space for quasiparticle scattering, and leads to the sizable suppression of the hot quasiparticle scattering rate found below T_* [7].

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